



U.S. Food and Drug Administration
Protecting and Promoting Public Health

www.fda.gov

Scope of Database



Substances

- Any substance intentionally added to a medicinal product
 - Priority
 - Active Substances and Active Moieties
 - Excipients
 - Impurities and Degradants
 - Metabolites (Out of Scope 11238; but will capture)
 - Specifications (Group 4 moved up capture Pharmacopeial Specifications at Group 3?)
 - Constituents of Complex Materials
 - Processing Materials (Specified Substances Group 4)
 - Synthetic Pathway (Group 4)
 - Targets (Therapeutic, Transporters, Metabolic Enzymes)



Data to be linked to Substances

- Names
 - Primary Name (INN English Name with Explicit Stoichiometry)
 - Official Names
 - Domain
 - Jurisdiction
 - Language
 - Chemical Names
 - Company Codes
 - Brand Names



Data to be linked to Substances

- Codes (Code System)
 - UNII
 - CAS Numbers (Chem ID)
 - INCHI Key
 - Pubchem CID
 - EINICS
 - Swiss Medic Codes
 - ASK Numbers
 - EVMPD numbers
 - Canadian codes
 - Other Regulatory codes



Data to be linked to Substances

- Relationships
 - Parent-Salt/Hydrate
 - Active Moiety
 - Prodrug-Active Metabolite
 - Parent-Active Metabolite
 - Parent-Less Active Metabolite
 - Parent-Metabolite
 - Parent-Inactive Metabolite
 - Parent-Impurity
 - Parent Degradent



Data to be linked to Substances

- Relationships
 - Parent-Salt/Hydrate
 - Active Moiety
 - Prodrug-Active Metabolite
 - Parent-Active Metabolite
 - Parent-Less Active Metabolite
 - Parent-Metabolite
 - Parent-Inactive Metabolite
 - Parent-Impurity
 - Parent Degradent



Data to be linked to Substances

- Relationships
 - Parent-Active Isomer
 - Parent-Inactive Isomer
 - Agonist-Target
 - Inhibitor-Target
 - Inducer-Target
 - Constituent (Always Present)-Parent
 - Constituent (May Be Present)-Parent



Data to be linked to Substances

- Relationships
 - Parent-Active Isomer
 - Parent-Inactive Isomer
 - Parent-Target
 - Parent-Transporter
 - Parent-Metabolic Enzyme
- Classification Systems
 - FDA Established Pharm Class
 - ATC
 - MESH
 - Chemical Classification



Data to be linked to Substances

- Properties Substances Level

- Molecular Weight
- Molecular Formula
- Spectra
 - Mass Spectra
 - NMR
 - IR
- Synthesis
- Biological Properties
 - Toxicity
 - Acute
 - Chronic
 - Developmental
 - Genotoxicity
 - Carcinogenicity
 - Organ Specific Toxicity



Data to be linked to Substances

- LADMER Data
 - BCS classification
 - Solubility
 - Dissolution
 - CACO cell data
 - Cmax
 - Oral Bioavailability
 - Tissue Distribution (Vd)
 - Blood Brain
 - Excretions
 - Response (Targets)
 - Protein Binding



Data to be linked to Substances

- Product Data and Application Data
 - Formulation (Ability to Capture and Enter)
 - Role of ingredients
- When MPID is implemented
 - Clinical Particulars
 - Indications
 - Contraindications
 - Interactions
 - Adverse events



Data to be Linked to Specified Substances for Chemicals

- Chemical Specified Substances
 - Used to capture ingredients that contain multiple substances (I.E. flavors; colorants)
 - Qualitative and Quantitative Information
 - Different polymorphic forms
- Physical form
 - Polymorphism
 - Solubilities
 - Melting Point
 - Particle Size